ALTERNATIVE METHOD FOR THE THERMOSPHERIC ATOMIC OXYGEN DENSITY DETERMINATION

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ABSTRACT

Atomic oxygen density in the upper thermosphere (~300 km) can be calculated using ground based incoherent scatter radar and Fabry-Perot interferometer measurements. Burnside et al. (1991) was the first to try this method, but Buonsanto et al. (1997) provided an extensive treatment of the method in 1997. This paper further examines the method using 46 nights of data collected over six years and the latest information on the oxygen collision frequency. The method is compared with the MSIS-86 atomic oxygen prediction values, which are based upon *in situ* rocket born and satellite measurements from the 70's to the mid-80's. In general, the method supports the MSIS-86 model, but indicates several areas of discrepancy. Furthermore, no direct correlation is found between the geomagnetic conditions and the difference between the method and MSIS-86 predictions.

INTRODUCTION

Due to its extreme height, elusiveness has often pervaded study of the thermosphere. In this respect, measurement of neutral atomic oxygen density ([O]) has been no different. The lack of constant data has forced researchers to rely upon the MSIS-86 model for calculations requiring thermospheric oxygen densities. While Hedin's (1987) model has proven to be generally reliable, it has limits and significant error margins. Buonsanto et al. (1997) estimated a 20% uncertainty for MSIS predictions in the higher thermosphere based on Hedin (1987). Burnside et al. (1991) found large errors during geomagnetically disturbed periods above Arecibo at 300 km with measured densities twice the predictions. Schoendorf and Oliver (1998) discovered underestimates in the MSIS predictions for years of maximum solar flux and overestimates for years of low solar flux at approximately the 400 km height (personal correspondence with Oliver) above the EISCAT observatory in Norway.

Such uncertainties for [O] predictions are unsatisfactory because atomic oxygen plays an important role in various thermospheric reactions. At an altitude of 300 km, neutral atomic oxygen constitutes roughly 80% of the total density of the atmosphere. Here it moves solar energy deeper into earth's thermosphere by transferring an electron through strong resonance charge exchange interaction with O⁺, providing the principal method of heating the thermosphere (Omidvar et al., 1998).

A new technique for determining [O] at about 300 km using ground based incoherent scatter radar (ISR) and Fabry-Perot interferometer (FPI) measurements was introduced by Burnside et al. (1991) using data collected at Arecibo. Buonsanto et al. (1992) provided a fuller treatment of the technique at Millstone Hill for fourteen nights of data ranging from March 19, 1990 to May 16, 1991. In this paper, we will further examine this technique for 46 nights with a larger data set, a greater span of time, and the most recent information on O-O collision frequency.

DATA COLLECTION AND INSTRUMENTATION

The data selected provides a wide spectrum of solar and geomagnetic activity. The data set includes 46 nights and 899 points of coincident ISR and FPI measurements from Aug. 19, 1988 to Mar. 3, 1995 at Millstone Hill

Observatory in Massachusetts, USA (42.6° N and 71.5° W). Almost every possible Kp value from 1 to 8- is represented within this selection. Buonsanto et al. (1997) originally processed the data.

By employing Thomson backscatter from ionospheric electrons, the incoherent scatter radar (ISR) is able to ascertain ion velocity along the magnetic field (V_0) , ion (electron) density (N_1) , ion temperature (T_2) , and electron temperature (T_2) . The Fabry-Perot interferometer (FPI) observes the atomic oxygen at 630 nm and calculates the neutral wind velocity (U) by reading the Doppler shift of the nightglow. Although the FPI can also provide neutral temperature measurements, these tend to have large uncertainties, making them less reliable than the radar measurements. The ISR is able to operate nearly continuously, but poor visibility from cloudy nights limits data from the FPI.

By combining the ISR electron density profile with data from the MSIS-86 model, the altitude of the maximum 630 nm emissions was estimated for each data point (Link and Cogger, 1988). It is at this altitude that the FPI makes its neutral wind velocity (U) readings, so all ISR data was selected for this altitude. Furthermore, the MSIS-86 atomic oxygen density predictions were also based upon this altitude. The maximum emission altitude tends to range about 50 km on any one night and may be as low as 250 km or as high as 350 km. It is generally about 300 km.

For more information on the data collection and instrumentation, we recommend Sipler et al. (1991) and Buonsanto et al. (1997). Sipler provides a complete discussion of the FPI and a summary of the ISR, and both Sipler and Buonsanto nicely overview the data collection for substantial portions of the same data used in this study.

THEORY: FROM DIFFUSION VELOCITY TO OXYGEN DENSITY

The diffusion velocity of the ions (W) can be calculated through two different forms:

$$W = U\cos I - V_{\parallel} \tag{1}$$

$$W = -\frac{2kT_p}{m_i v_{in}} \left[\frac{1}{N_i} \frac{\partial N_i}{\partial z} + \frac{1}{T_p} \frac{\partial T_p}{\partial z} + \frac{m_i g}{2kT_p} \right] \sin I$$
 (2)

where $T_p = (T_i + T_e) / 2$ is the plasma temperature, U the horizontal meridional neutral wind velocity, I the magnetic dip angle, V the ion velocity along the magnetic field, k the Boltzmann constant, m_i the ion mass, v_{in} the ion-neutral collision frequency, N_i the ion (electron) density, z the altitude, and g the acceleration due to gravity (Reddy et al., 1994). It is assumed that the ionosphere is composed of O^+ , so all calculations refer to this ion.

The theoretical collision frequency, including the minor contributions of $[N_2]$ and $[O_2]$, is given by:

$$V_{in}^{th} = Q_d^{th}[O] + 6.9 \times 10^{-16}[N_2] + 6.7 \times 10^{-16}[O_2], \tag{3}$$

where Q_d^{th} is the theoretical momentum transfer collision cross section of O^+ -O and contributions of $[N_2]$ and $[O_2]$ are obtained using Banks (1996) and MSIS-86 predictions.

Three sets of calculations by Stubbe (1968), Stallcop et al. (1991), and Pesnell et al. (1993), provide consistent values of Q_dth within a few percent of each other. The formula by Pesnell et al. is given by:

$$Q_d^{th} = 3.0 \times 10^{-17} T_r^{1/2} (1 - 0.135 \log T_3)^2$$
 (4)

where $T_r = (T_i + T_n) / 2$, with T_n the neutral temperature and $T_3 = T_r / 1000$. Pesnell's values for the Q_d^{th} of [O] are larger than the commonly used values of Dalgarno (1964) by 1.38, 1.32, 1.28, 1.24, and 1.22 at 500 K, 750 K, 1000 K, 1250 K, and 1500 K respectively.

The quest for empirical verification of Q_d started roughly, but has began to come into focus. Burnside et al. (1987) used ISR and FPI data from Arecibo to calculate v_{0-0} , but his values were 1.7 times larger than those predicted by Dalgarno. Sipler et al. (1991) used a similar technique at Millstone Hill to calculate values 1.9 times larger than Dalgarno, and Salah (1993) recommended an official correction value of F = 1.7, which was termed the Burnside Factor.

In the next few years, a series of papers found fault with the previous data analysis methods. Reddy et al. (1994) demonstrated a systematic overestimate of Q_d from errors in the measurements. Hines et al. (1997) questioned the use of the least-squares method in this application. Buonsanto et al. (1997) conducted Monte Carlo simulations on Millstone Hill data, discovered a systematic overestimate from random errors, and calculated an unbiased $F \approx$

1.4±0.3. Finally, Omidvar et al. (1998) conducted three different analysis methods on the Millstone Hill data and determined the data supported the theoretical formula by Pesnell et al.

A new experimental measurement of O⁺-O charge-exchange cross section has recently been reported by Lindsay et al. (2001). In this work, electron capture cross section by the pure ground states of O⁺ has been measured, while in the previous works cross sections are due to a mixture of the ground and the contaminated excited states of O⁺. When compared with the measurements of Stebbings et al. (1964) we find the cross sections increase by a factor of 1.1 at impact energies of 5000eV and a factor of 1.5 at impact energies of 500 eV. Unfortunately, these energies are well above the energies of our interest, so no conclusion can be drawn on the correct values of the cross section at thermal energies. However, this new result generally questions the accuracy of the collision frequencies currently being used by workers in the field.

By using the calculation of the diffusion velocity from Eq. 1 and combining Eqs. (2) and (3), we arrive at the following formula:

$$W = \frac{-\frac{2kT_p}{m_i} \left[\frac{1}{N_i} \frac{\partial N_i}{\partial z} + \frac{1}{T_p} \frac{\partial T_p}{\partial z} + \frac{m_i g}{2kT_p} \right] \sin I}{Q_d^{th}[O] + 6.9 \times 10^{-16} [N_2] + 6.7 \times 10^{-16} [O_2]}.$$
 (5)

We introduce

$$\gamma = -\frac{2kT_p}{m_i} \left[\frac{1}{N_i} \frac{\partial N_i}{\partial z} + \frac{1}{T_p} \frac{\partial T_p}{\partial z} + \frac{m_i g}{2kT_p} \right] \sin I$$
 (6)

and

$$V_{correction} = 6.9 \times 10^{-16} [N_2] + 6.7 \times 10^{-16} [O_2]$$
 (7)

Then Eqs. (5), (6), and (7) can be used to determine the neutral atomic oxygen density as such:

$$O = \frac{D}{W} \tag{8}$$

where

$$D = \frac{\gamma - W V_{correction}}{Q_d^{th}}, \tag{9}$$

where O is the neutral atomic oxygen density, γ groups many of the terms from Eq. (2), $v_{\text{correction}}$ accounts for the $v_{\text{O--}}$ and $v_{\text{O--}O2}$, W is the diffusion velocity from both ISR and FPI wind data, and D is the theoretical portion from ISR temperature data.

ANALYSIS

The past two studies of atomic oxygen density by Burnside et al. (1991) and Buonsanto et al. (1992) used a correction factor F = 1.7 and Dalgarno's formula for Q_d . Based upon Omidvar et al. (1998), the present work uses a correction of F = 1.0 and Pesnell's formula for Q_d . We have adjusted all of Buonsanto's data accordingly.

The original 899 data points encompass an extreme range of values. Data collected by these instruments is prone to be disordered. This is the primary reason past studies have had difficulty in ascertaining the collision cross section. We remove outliers by only accepting points producing F values between 0.35 and 3.0. Values outside this boundary (1/3 of MISS-86 [O] predictions to 3 times MISS-86 [O] predictions) are highly unlikely.

After removing the outliers, the data set has 786 points. Figure 1 displays this data and the boundaries of outlier rejection. Each point consists of a D, W, and O. The D and W are derived from empirical data, while the O is the MSIS-86 [O] prediction for the particular time, position, and altitude of the matching data. In a perfect world, the MSIS derived [O] will equal the D/W derived [O], so we compare these two values to check the accuracy of using ISR-FPI data to measure [O] and check the validity of the MSIS model.

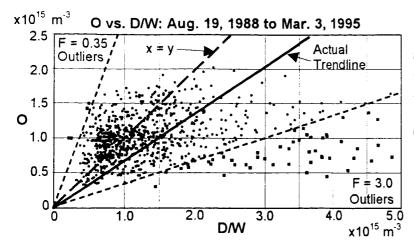


Fig. 1. This plot shows the 786 data points (circles), the boundaries of outlier exclusion (lines with short dashes), and outliers (squares). An additional 61 outliers lay off the right side of the chart.

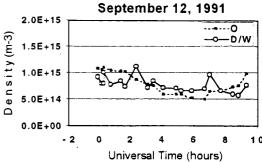


Fig. 2. This chart plots the measured D/W and the predicted O versus the time the data was taken. Each O prediction is based upon the estimated altitude the D/W was measured. The measurements vary in altitude, which manifests itself as fluctuations in the O predictions.

If the O's are a close match to the D/W's, we would expect the data to group about the x = y trendline shown in Figure 1. Although a third of the data points do group about this line, a large number of data points diverge: 257 of the D/W data points are within 20% (an estimated error of MSIS predictions) of the O, but 185 have a difference of 20% or lower and 344 have a difference of 20% or higher. In essence, D/W's are heavily skewed toward the right side and have a wide data spread (Table 1) approximating a lognormal distribution. This skew of the data pulls the actual least-squares trendline downward. In contrast, the MSIS-86 O predictions form a Gaussian distribution.

Perhaps the best analysis of the data is on a night by night basis. Twenty-four nights have average percent differences of the absolute value between D/W and O greater than 40%. On a few of these nights, the data is extremely erratic, with abrupt changes of around 100% resulting from both dramatic shifts in wind speed and large changes in D. A number of nights display consistently different trends from MSIS-86 predictions. Nonetheless, data from eight nights closely follows MSIS predictions. One of the best examples is September 12, 1991 (max Kp 3-), which has an average difference of 21.2% and a significant correlation coefficient of 0.503 (Figure 2).

We found no significant positive correlation between the geomagnetic activity and the average percent difference between D/W and O (Figure 3). For example, April 10, 1990 exhibits an average density approximately twice the MSIS-86 predictions during a geomagnetic storm with a max Kp of 8-, but so does January 26, 1995 even though it maintains a low Kp of 1. This is somewhat in contrast to Burnside et al. (1991) who suggested densities dramatically increased above MSIS-86 predictions during geomagnetically disturbed periods based upon measurements on July 14, 1985 (max Kp 4+) and January 15, 1988 (max Kp 7+).

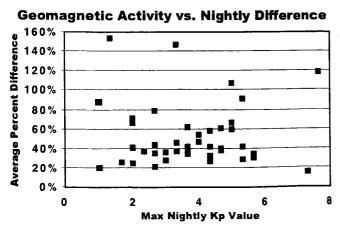


Fig. 3. No statistically significant trend appears in a comparison of the geomagnetic activity and the average absolute nightly difference between O and D/W.

Over half of the data was collected from Aug. 19, 1988 to September 21, 1990. This concentration of twenty-six nights over two years allows the opportunity to search for seasonal trends. We average each night of data to approximate the atomic oxygen density for that period of the year. Figure 4 shows a clear seasonal cycle with a winter maximum and summer minimum. In general, the alternative method produces averages larger than the MSIS-86 predicted averages.

Table 1. Statistical Information (SD = Stand. Dev.)

Data	Mean	Median	SD/Mean
0	1.02x10 ¹⁵	9.80x10 ¹⁴	31.4%
D/W	1.24x10 ¹⁵	1.08x10 ¹⁵	52.8%

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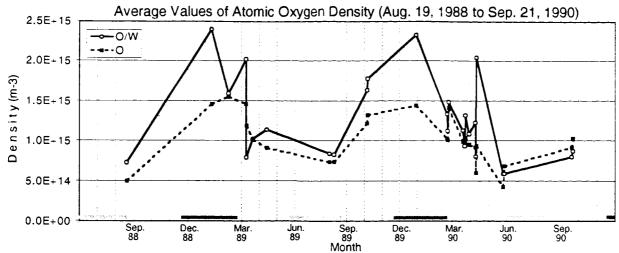


Fig. 4. Average nightly values of D/W and O data. The dark bars at the bottom of the graph show the winter season, while the lighter bars show the summer season.

velocities (ion velocity from the ISR and the neutral wind velocity from the FPI) will have the largest effect upon the results. Both of these velocities factor into the calculation of the diffusion velocity (W). Buonsanto et al. (1997) states that both items have random instrumental errors of 20% or more. Furthermore, he demonstrated that random errors will skew data to the right when W is in denominator, inflate the oxygen density values when the errors are large, and raise the average oxygen density but leave the median density unaffected. Indeed, our results show the average value of the D/W's is 22 % larger than the average for the O's, but the median is only 10% larger (Table 1).

Additionally, the FPI neutral wind measurements will be influenced if vertical winds are present because the FPI uses the vertical direction as a zero reference with the assumption vertical winds are negligible. A study by Sipler et al. (1995) on nighttime vertical winds above Millstone Hill revealed downward movement on the order of 10 m/s with little variability on geomagnetically quiet nights (Kp≤3) and radically varying movement with a possible oscillatory nature on the order of 20 m/s to -50 m/s on geomagnetically active nights (Kp>3). If a geomagnetically calm night has a consistent downward wind, it would manifest itself as a systematic error consistently lowering the results below reality. During geomagnetically disturbed periods, when vertical winds may be large and highly variable from a negative to positive direction, the results can be seriously changed.

Other errors may include: 1. the uncertainty of the atomic oxygen collision frequency at thermal energies, and 2. a nonuniform ion velocity field. The effect of error on the data has a close correlation to the magnitude of the diffusion velocity, as seen in Figure 5. The higher velocities tend to have negative differences, while the lower velocities have large positive differences. The difference between O and D/W is highly sensitive to errors that decrease the size of low diffusion velocities. As errors force W to zero, D/W goes to infinity. In fact, ninety-six percent of the outliers removed had diffusion velocities below 20 m/s.

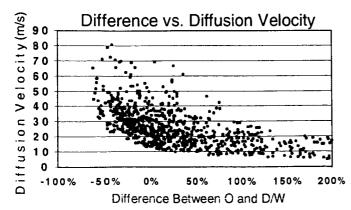


Fig. 5. A clear correlation: The differences between the O's and the D/W's increase as diffusion velocity decreases.

CONCLUSION

The random instrumental errors, the exclusion of vertical winds, and the intrinsic error margins within the MSIS-86 model provide a caution on any conclusions made concerning the data. With this in mind, we believe the eight nights of data which closely matches MSIS-86 predictions, the grouping of a third of the data points within the error margins of the MSIS-86 model, and the similarity between the medians of the D/W's and O's suggest the data generally supports the MSIS-86 model. There were a number of nights that displayed consistently different trends from the MSIS-86 model. These indicate needed refinement in the MSIS-86 model and suggest greater variability in the magnitude of the atomic oxygen density than predicted.

In an interesting result, geomagnetic activity does not appear to have a simple one-to-one impact upon the average difference between MSIS-86 predictions and the alternative method. This is contrary to the belief the MSIS-86 model will have a greater difference from reality during geomagnetically disturbed nights and indicates large errors can enter the data on quiet nights as well as disturbed nights.

In conclusion, employing ISR and FPI data to calculate atomic oxygen density in the higher thermosphere provides a ground based method to monitor changes. Unfortunately, it is prone to large errors and requires simultaneous measurements from unique equipment available at only a few locations in the world. Further study on vertical winds would improve the accuracy of the data. Although limited by these factors, this method has the benefit of allowing detailed, long-term study of upper thermospheric nighttime atomic oxygen density. This major benefit encourages continued, although cautious, use of this method.

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Popular Summary of the Manuscript "Alternative Method of the Thermospheric Atomic Oxygen Density Determination"

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The *in situ* satellite measurement of the thermospheric atomic oxygen density is in error by 20 to 40% of the actual values. An alternative ground based, compared to *in situ*, measurement is to find this density through the equation of force balance, involving the gravitational and magnetic forces acting on neutral and charged particles in the thermosphere.

Parameters appearing in the equation of force balance needed to determine the oxygen atom density are particle neutral velocity, ion velocity along the magnetic lines of force, ion and electron densities, and ion and electron temperatures. All these parameters can be found by the ground based radar, except the particle neutral velocity which is found by the Fabry-Perot interferometer. In addition, the collision frequency between O⁺ and O is needed, whose accurate values have recently been obtained by several detailed quantum mechanical calculations.

In this paper, we make use of the equation of force balance, 46 nights of the needed data, collected over six years at the MIT Millstone Observatory, and the calculated values of the collision frequency, to determine the atomic oxygen density. When compared to the MSIS-86 Model, which is based on *in situ* rocket born and satellite measurements, the alternative ground based method supports the *in situ* MSIS-86 model, but indicates several areas of discrepancy. We have also found a weak correlation between the oxygen atom density and intensity of the solor magnetic storms.